

# Cyclohexylaminoacetonitrile

<b>Inchi:</b>	InChI=1S/C8H14N2/c9-6-7-10-8-4-2-1-3-5-8/h8,10H,1-5,7H2
<b>InchiKey:</b>	PIYOTHVPNLMMFD-UHFFFAOYSA-N
<b>Formula:</b>	C8H14N2
<b>SMILES:</b>	N#CCNC1CCCCC1
<b>Mol. weight [g/mol]:</b>	138.21
<b>CAS:</b>	1074-58-4

## Physical Properties

Property code	Value	Unit	Source
gf	263.50	kJ/mol	Joback Method
hf	64.22	kJ/mol	Joback Method
hfus	14.92	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.432		Crippen Method
mcvol	124.080	ml/mol	McGowan Method
pc	3110.57	kPa	Joback Method
tb	554.24	K	Joback Method
tc	777.41	K	Joback Method
tf	304.95	K	Joback Method
vc	0.477	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.89	J/molxK	554.24	Joback Method
cpg	318.10	J/molxK	591.44	Joback Method
cpg	332.38	J/molxK	628.63	Joback Method
cpg	345.75	J/molxK	665.83	Joback Method
cpg	358.26	J/molxK	703.02	Joback Method
cpg	369.93	J/molxK	740.22	Joback Method
cpg	380.78	J/molxK	777.41	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074584&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074584&amp;Units=SI</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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